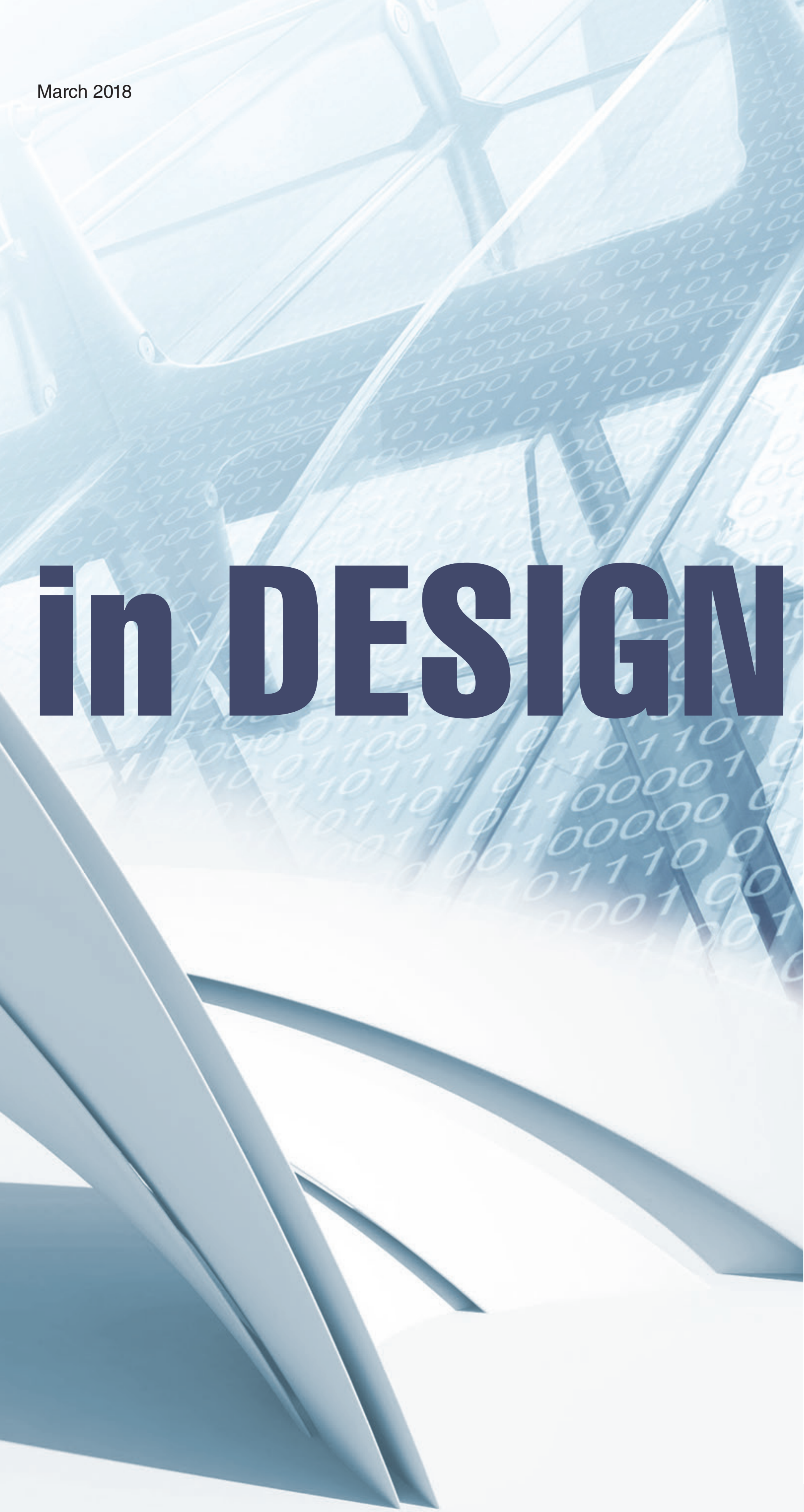
LEADING A REVOLUTION

Livermore researchers are creating powerful software for designing objects previously unobtainable.



in DESIGN

ADDITIVE manufacturing technologies—often called three-dimensional (3D) printing—represent a revolution in how products are made. Now being adopted by U.S. industry, the approach allows an extreme level of control over shape and material composition at scales down to nanometers, creating the potential to engineer materials with desired structural, thermal, electrical, chemical, and photonic properties in a single package. Novel structures having complex microarchitectures and composed of metals, polymers, and ceramics are being created. In some cases, multiple materials are combined to create "metamaterials" with properties never before possible.

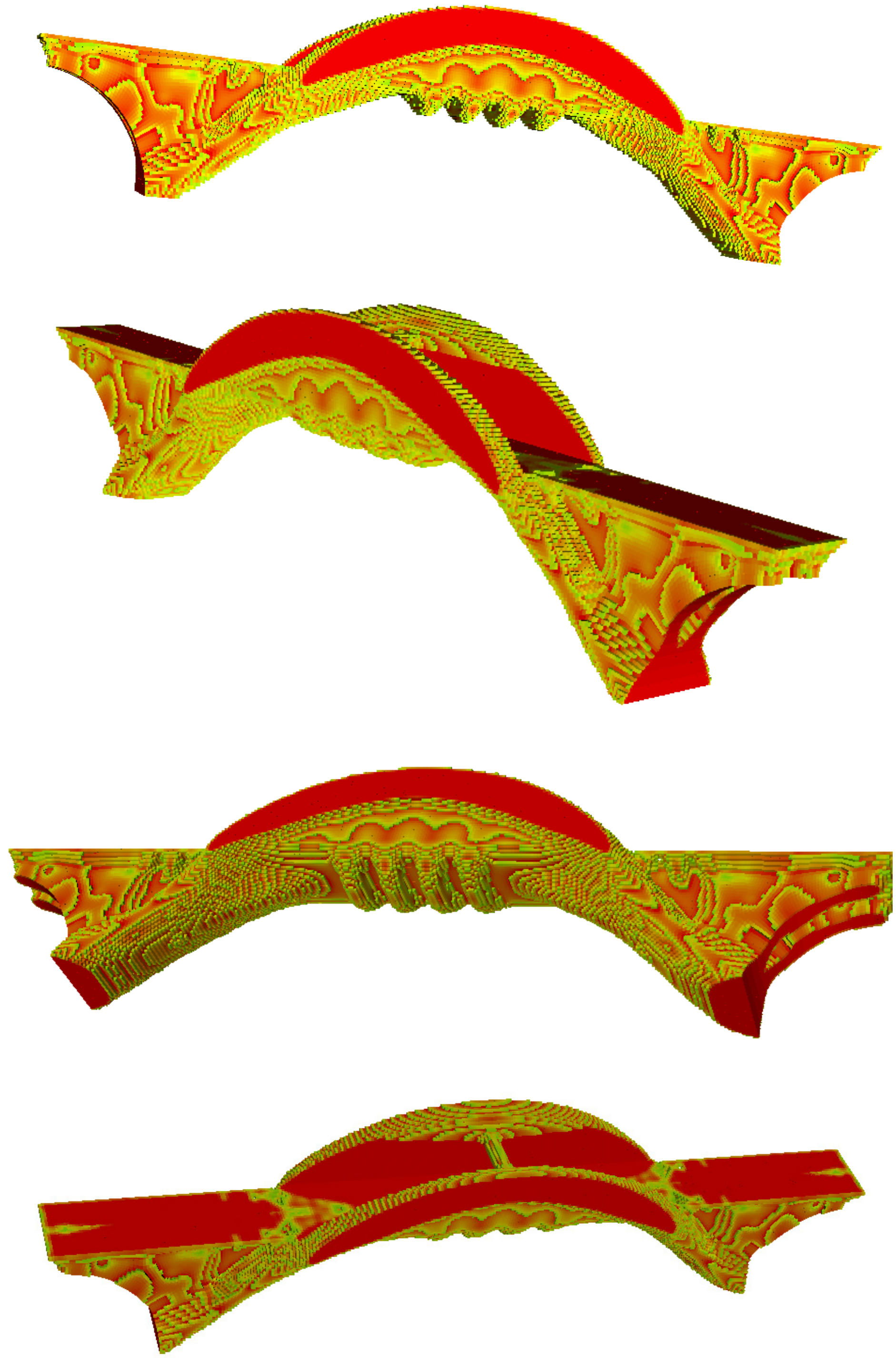
Engineers and computer scientists at Lawrence Livermore are working together to produce new materials with additive manufacturing, drawing on expertise in precision engineering, highly detailed computer modeling and simulations, materials science, and high-performance computing (HPC). The new parts and systems, intended for Livermore's national security missions, offer greater performance, reduced time to manufacture, less waste, and often lower cost.

Because additive manufacturing eliminates many previous manufacturing constraints, engineers are beginning to rethink design basics and how to achieve products with greater complexity and enhanced performance. However, without formal design paradigms that take full advantage of the technique's potential, researchers currently generate designs for additive manufacturing using a costly trial-and-error approach based on conventional design tools such as computer-aided design and computer-aided engineering (CAE) software, guided solely by the engineer's experience and intuition. Such practices all too often result in only incremental improvements to existing designs.

Replacing Trial and Error

Mechanical engineer Dan Tortorelli, who leads the Laboratory's Center for Design Optimization, is working to fundamentally transform how engineers design complex parts and systems to be additively manufactured. Tortorelli says, "Our ability to manufacture exceeds our ability to design. Design has become a bottleneck, in that designing a part for additive manufacturing is sometimes more difficult than actual fabrication." Engineers can face a bewildering number of possible designs when striving for the necessary combination of nonlinear, transient, multiscale, and multiphysics attributes in a part or system. "The opportunity and need to fundamentally transform design is one of the most compelling frontiers in engineering," says Tortorelli. "We want to give engineers the tools to help them rethink what is possible. New shapes with new internal structures that would have been prohibitively costly or even impossible to manufacture only a few years ago are now possible."

Tortorelli states that conventional design methods and computer algorithms are constrained by outdated presumptions about material properties and manufacturing methods and do not take advantage of the modeling and simulation capabilities, data analytics, and algorithms that are common in HPC. As an example he compares a modern-day composite airplane fuselage to a centuries-old wooden ship. Except for modern materials, the designs are strikingly similar. In short, simply using



This projection shows a 60-meter-long bridge designed by Livermore Design Optimization (LiDO) software. The design inputs for LiDO included a "bounding box" to fill with material and a load distribution representing car weight. The design is optimal in that for a given weight, stiffness is the maximum possible. To enhance stiffness, the design features four ribs on the bridge's underside and a cross member between the arches.

additive manufacturing to fabricate products designed with conventional techniques misses the point. Chris Spadaccini, director of Lawrence Livermore's Additive Manufacturing Initiative, adds, "Without a proper HPC-based design framework, engineers risk leaving much manufacturing capability on the table. Control of microarchitecture offers the potential for materials designed with new functionalities and an order-of-magnitude improvement in performance." (See the box on p. 10.)

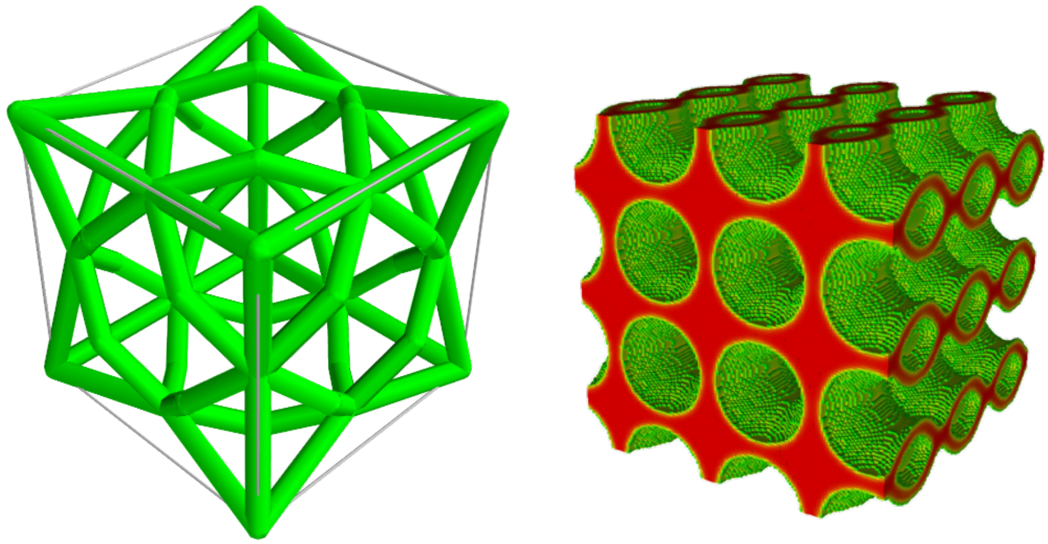
Leveraging Computation

The Center for Design Optimization was established in October 2016 in response to the critical need for a comprehensive computing environment that takes full advantage of additive manufacturing. With funding from the Laboratory Directed Research and Development Program, the center launched a three-year Computational Design Optimization Strategic Initiative led by principal investigators Tortorelli and computational engineer Daniel White. In this effort, more than a dozen Livermore computer scientists and engineers are leveraging the Laboratory's extensive HPC capabilities to develop an efficient design optimization software package called Livermore Design Optimization (LiDO). Collaborators include researchers from the University of Illinois; Lund University, Sweden; the University of Wisconsin; the University of Texas at Austin; Technical University, Denmark; the International Computing Science Institute, in Berkeley, California; and CAE software firm Autodesk, Inc., based in San Rafael, California.

The team's goal with LiDO is to provide a cohesive design environment where Livermore's rapidly growing additive manufacturing capabilities are seamlessly combined with HPC resources such as codes, algorithms, powerful modeling and simulation tools, data analytics, and some of the world's most powerful supercomputers. The fully integrated LiDO combines multiple length scales, geometric representations, multiresolution capability, multiphysics, and uncertainty factors for optimizing designs characterized by transient and nonlinear phenomena. LiDO systematically traverses the design space to obtain the shapes and microarchitectures that best meet the requirements specified by the user.

Rob Sharpe, deputy associate director for research and development in Livermore's Engineering Directorate, tells how managers in the directorate began to think about the need to transform design work as colleagues began investigating, adopting, and inventing additive manufacturing processes as part of Engineering's Advanced Materials and Manufacturing Initiative. "We began to explore the possibility of first describing the desired functions of a new part—such as the size and properties—and then turning the computer loose to arrive at the best design."

This design for a drone chassis with four rotors accommodates two different loads—the upward force of the rotors and the downward pull of gravity, especially on the camera and batteries. Design optimization with LiDO software required Livermore's Vulcan supercomputer and used 100 million mesh elements—well beyond the capability of commercial software.



Two examples of unit cells, the basic component of an additively manufactured part or system, are shown. Both are designed for maximum stiffness and are of arbitrary dimensions. Aggregates of these cells can form microtrusses to serve as building blocks for much larger structures, ranging from bridges to antennas.

Tortorelli says, "We want to enable the design of systems that were previously unobtainable, unthinkable, and unimaginable." By providing the best design tools, the LiDO development team anticipates nonintuitive, high-performing designs for Laboratory missions in national and global security, lasers, and energy. The code takes into account a host of objectives such as weight, volume, and manufacturability. Ensuring manufacturability enables an engineer to consider only those designs that are readily buildable. Collaborating researchers at the University of Wisconsin are working to quantify manufacturing uncertainty and ensure robust designs that are resistant to defects.

Liberating Engineers

Sharpe points out that Livermore engineers are often charged with design tasks that go far beyond intuition because of their scale and complexity. An engineer can confidently understand the forces that a static object such as a solid bridge must withstand and test the object virtually for its response to these forces. However, intuition is severely limited when thinking about structures that operate in the nonlinear regime or when many different physics are involved. For example, a part may have to take into account a combination of structural, thermal, optical, and electrical phenomena, ranging from the speed of sound to the speed of light. A part may need to absorb a sudden compressive force and then spring back to its original shape, compress less and less as a force increases, or deliberately fail when compression exceeds a certain point. "At the Laboratory, we often need designs for systems that undergo large deformations," explains Sharpe. "We need to know how they will respond in nonlinear situations." Examples in everyday life include a bicycle helmet that fractures as designed during a violent impact, and a car bumper that returns to its original shape when lightly tapped but crumples extensively in a high-speed accident.

"It is difficult for a classically trained engineer to conceptualize all the possible shapes that solve a problem, especially radically new designs," observes White. As an example of the potential design burden, additive manufacturing permits the placement of a different material at every corner of a repeating microtruss, which itself can vary in size, degree of stiffness, and other structural properties. As a result, the number of possible design options quickly approaches infinity, making any trial-and-error process to produce an optimized object a daunting proposition.

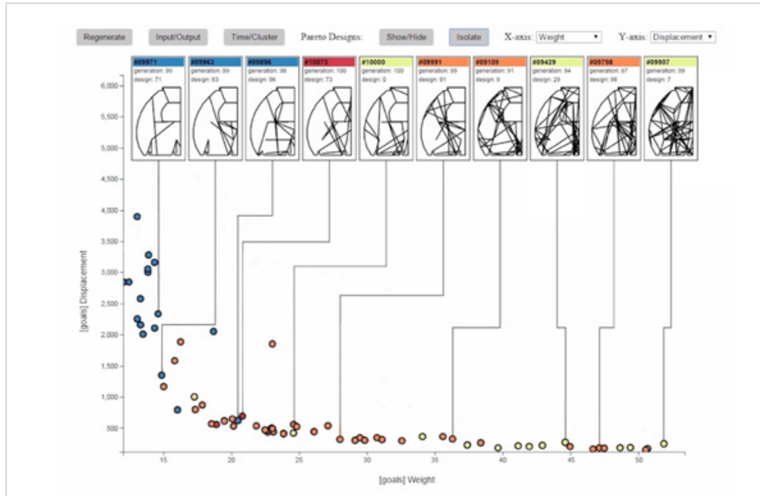
White states that LiDO can liberate engineers from trial and error and the overwhelming design choices afforded by additive manufacturing. Currently, an engineer uses various software packages to create a prototype design and subsequently simulates the desired output, such as calculated mass and the stress and strain such a shape would likely experience. The engineer then determines whether the design meets the prescribed specifications. If not, the process is repeated with a revised design. LiDO reverses the process: An engineer compiles a list of desired mass and maximum stress and strain levels, after which LiDO determines the final shape and internal microstructure. Letting HPC do the hard work saves weeks of development time.

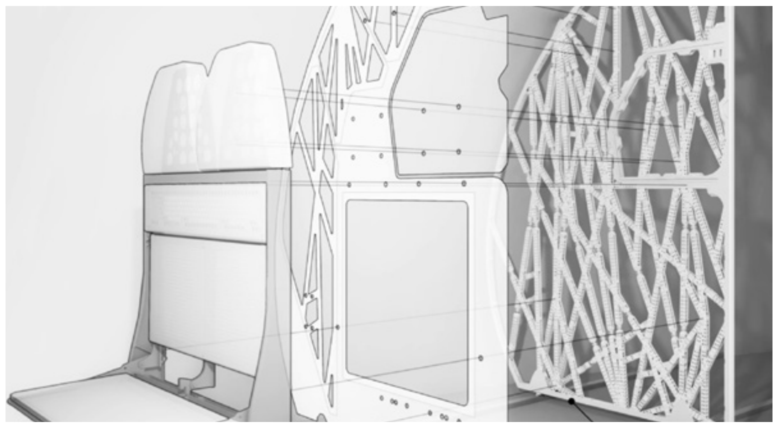
Leveraging Current Software

LiDO is massively parallel, meaning the software is designed to run on a supercomputer that uses a large number of processors simultaneously. In fact, LiDO builds upon existing software developed by Livermore's Computation Directorate for solving huge physics problems on large parallel supercomputers such as the Laboratory's Sequoia supercomputer, which is capable of speeds of up to 20 petaflops (one quadrillion floating-point operations per second). LiDO uses a software resource called MFEM (Modular Finite Element Methods), a Livermore-developed open-source, scalable software library for converting real-world physics problems into discrete computational representations based on finite elements—meshes of squares, cubes, triangles, or tetrahedrons—and solving the resulting simultaneous equations, which number in the hundreds of millions. LiDO also leverages Livermore's HYPRE library of linear solvers to enable larger, more detailed scientific simulations by solving problems more quickly than traditional methods can. HYPRE has been used by research institutions and private companies to simulate phenomena such as groundwater flow, magnetic fusion energy plasmas, blood flow through the heart, and pumping activity in oil reservoirs.

Tortorelli explains that commercially available design optimization software is limited primarily to simple physics and assumptions of linear and static behavior. Because of the small customer base, software vendors are not motivated to incorporate the complex, nonlinear physics that Livermore researchers must consider in their design problems. Academic researchers may tackle more complex design optimization problems than industry does, but few universities have at their disposal the immense supercomputer facilities needed to run integrated design optimization software.

LiDO is not expected to be finished until 2019, but researchers are already demonstrating many of its design capabilities. One emphasis is demonstrating new designs for strong, lightweight structures that require reinforcement at high-stress spots. "Such design freedom is not available with commercial software," says White. "With LiDO, we do not have to make a part uniform. We can tailor the material architecture to accommodate varying stress levels." White notes that historically, more than 99 percent of all design optimization problems involve maximizing stiffness, and so LiDO developers are focusing on demonstrating efficient and original designs for structures such as bridges and drones. Their design solutions involve spatially varying microarchitected





Livermore industrial partner Autodesk, Inc., has used design optimization capabilities to design a partition panel for commercial passenger jets. (top) The software's user interface presents multiple options. (middle) The design chosen is shown integrated into existing structures. (bottom) The three-dimensionally printed metal partition panel is half as light yet just as strong, saving fuel and reducing carbon dioxide emissions.

lattices based on repeating unit cells for reduced weight and increased strength. For example, a simulated bridge that first appears to be a solid object is actually a series of repeating microtrusses, which vary in size and distribution to maximize the strength-to-weight ratio—that is, to effectively carry the load in high-stress regions but save weight in low-stress regions. This “lattice of lattices” approach is similar to that employed in the Eiffel Tower, a structure that was considered revolutionary for its novel design when built.

Many real-world design problems faced by Livermore researchers involve multiphysics, such as a part that must withstand both thermal and mechanical loads or be able to both reduce aerodynamic drag and absorb energy in an impact. LiDO’s multiphysics capabilities can be seen in the design of structural electromagnetic devices such as antennas that satisfy strength and stiffness requirements while only minimally attenuating electromagnetic waves. Optimized design variations for these devices feature silicon dioxide pillars composed of microlattices (for strength) topped with nanoantennas having tunable

Advancing Additive Manufacturing

For nearly a decade, Lawrence Livermore has been advancing the science of additive manufacturing. Also called three-dimensional (3D) printing, additive manufacturing uses a digital file to build 3D structures. Most additive manufacturing processes build up layers of material to precisely create objects with complex shapes engineered to handle a variety of forces. One well-established technique is direct ink writing, which deposits an ink made of silicone or other materials onto a substrate one layer at a time in a predetermined pattern. The resulting structure is then cured with heat or ultraviolet light.

By sequentially layering materials, additive manufacturing affords the ability to control both material composition and structure at multiple length scales and create objects with desirable material properties and performance. The process is being adopted by many industries to drastically reduce product development and production, particularly for low-volume specialty parts and tooling. Contrary to what the name might imply, the process actually requires less material than subtractive fabrication methods, such as machining or etching.

More than 100 material scientists, chemists, physicists, engineers, and computational scientists at Lawrence Livermore are participating in this effort to develop advanced materials and manufacturing processes. Examples include catalyst-filled beads to capture carbon dioxide from flue gas and new armor material for U.S. soldiers. Much of the effort is funded by the National Nuclear Security Administration (NNSA) in a multiyear program that is exploring and adapting the most promising technologies. The goal is to demonstrate the ability to produce complex parts with geometries that are unobtainable with conventional manufacturing methods, and with significantly less performance uncertainty.

Additive manufacturing is proving particularly valuable for stockpile stewardship, the NNSA program to ensure the continued safety, security, and effectiveness of the U.S. nuclear arsenal. The technique is helping to shrink the program’s manufacturing footprint and bring about more agile operations. Livermore researchers are also showing how additive manufacturing can improve both speed and quality in developing replacement parts, prototypes, test objects, and related materials. (See *S&TR*, January/February 2015, pp. 4–11.)

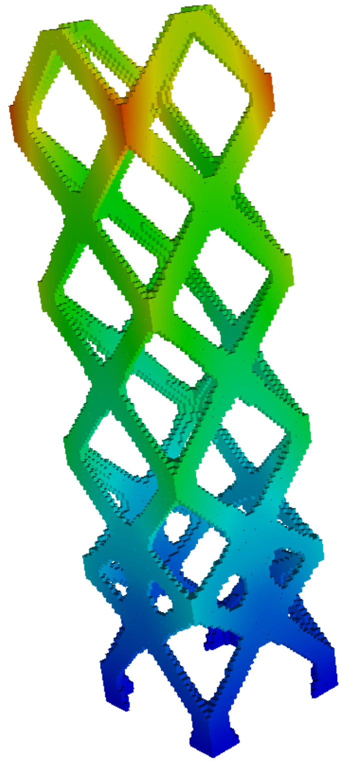
Materials scientist Chris Spadaccini, director of Livermore’s Additive Manufacturing Initiative, notes that of the dozen or so different additive manufacturing processes in use at the Laboratory, many were invented or improved upon by Livermore researchers. One example is digital holography, which reconstructs 3D geometrical information. The process was developed with researchers from the University of California at Berkeley and uses a diffractive optical element to phase-modulate a laser beam so that multiple images of a holographically shaped light field intersect in a volume of resin. Millimeter-scale parts with approximately100-micrometer resolution form in about 10 seconds without requiring a support structure. (See the article beginning on p. 12.)

Novel products with remarkable properties continue to be achieved by Livermore researchers. In late 2017, a team announced the 3D printing of composite silicone materials that are flexible and stretchable and possess shape memory behavior. The combination of 3D printing with shape memory characteristics is often referred to as four-dimensional printing, with the fourth dimension being time. The breakthrough could lead to innovations ranging from body heat–activated helmet cushions to form-fitting shoes. Also in late 2017, Livermore researchers and collaborators at Ames National Laboratory, Georgia Tech University, and Oregon State University 3D-printed a marine-grade stainless steel, achieving unparalleled strength and high ductility. The team plans to investigate producing high-performance steels and other lighter weight alloys.

The resounding success of Livermore’s additive manufacturing capabilities, along with increasing interest expressed by U.S. industry, spurred construction of the Advanced Manufacturing Laboratory (AML), a $10 million, 1,300-square-meter facility scheduled to open in early 2018. Located in the Livermore Valley Open Campus, AML is intended to foster partnerships between Livermore additive manufacturing experts and U.S. businesses. The facility houses the most advanced equipment in the field, including manufacturing, material evaluation, and characterization devices, along with high-performance computational modeling and simulation systems.

electromagnetic characteristics. These metamaterials can be engineered to be transparent to electromagnetic waves, to disregard only certain frequencies, or to be 100 percent reflective like a mirror.

Some shapes suggested by LiDO evoke curvatures and complex microstructural designs that are found in nature but which would be prohibitively difficult or expensive to fabricate with conventional manufacturing. These new shapes—called biomimetic—can resemble those found in living organisms. Sharpe points to mollusks whose shells have developed prodigious resistance to the attacks of predators. A cross section of such a shell resembles a brick wall with a staggered lattice architecture combined with pliable mortar. Another example is a species of shrimp that wields spines like tiny battering rams, with tremendous strength for their size.



An optimized design for a column that resists twisting is shown. Red represents the highest strain, blue the lowest.

Recognizing the Potential

Livermore's efforts are supported by the Defense Advanced Research Projects Agency (DARPA), which develops technologies for the Department of Defense and is looking to change the way the military models, designs, and manufactures its next-generation vehicles and weaponry. The agency's Transformative Design (TRADES) program funds development of algorithms that can take full advantage of new materials and fabrication methods. Jan Vandenbrande, DARPA program manager, explains, "The structural and functional complexities introduced by today's advanced materials and manufacturing methods have exceeded our capacity to simultaneously optimize all the variables involved. We have reached the fundamental limits of what our computer-aided design tools and processes can handle, and we need revolutionary new tools that can take requirements from a human designer and propose radically new concepts, shapes, and structures that would likely never be conceived by even our best design programs today, much less by a human alone."

In January 2017, DARPA awarded a four-year, multimillion-dollar TRADES grant to Lawrence Livermore, Autodesk, the University of California at Berkeley, and the University of Texas to develop advanced tools for not only generating designs with additive manufacturing but also for better managing the complexity of those design processes. Under the project, the Laboratory is developing algorithms capable of optimizing large, complex systems and working with Autodesk to create a user-friendly graphical interface. The ultimate goal is to help the Department of Defense design game-changing systems.

Tortorelli believes that LiDO will allow the tremendous potential of additive manufacturing to finally be realized. "We want to rethink and revolutionize design so that engineers have a clean design slate." He emphasizes that the software development effort is not aimed at taking engineers out of the design loop. Instead, he states, "We want to simplify their work and eliminate drudgery." Tortorelli expects the new design optimization paradigm to accelerate discovery and innovation, including the invention of new materials, objects, and systems with applications in the National Nuclear Security Administration's Stockpile Stewardship Program, energetic materials for defense uses, and high-energy-density target materials for fusion energy research at Livermore's National Ignition Facility. The effort will also likely inspire industry to more readily consider incorporating HPC to advance its own product development with additive manufacturing, thus advancing U.S. manufacturing as a whole.

Sharpe believes that LiDO is only an important first step in totally reinventing design. He sees another looming and intriguing aspect to the design process—incorporating aesthetics. He says, "Design is one of the frontiers of science and technology. It would be a travesty to use the same old designs with revolutionary new manufacturing technologies. Instead, we want to take full advantage of these new design capabilities, too."

—*Arnie Heller*

Key Words: additive manufacturing, Advanced Manufacturing Laboratory (AML), Advanced Materials and Manufacturing Initiative, Center for Design Optimization, Defense Advanced Research Projects Agency (DARPA), direct ink writing (DIW), four-dimensional printing, high-performance computing (HPC), HYPRE, Laboratory Directed Research and Development Program, Livermore Design Optimization (LiDO) software, MFEM (Modular Finite Element Methods), stockpile stewardship, three-dimensional (3D) printing, Transformative Design (TRADES) program.

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